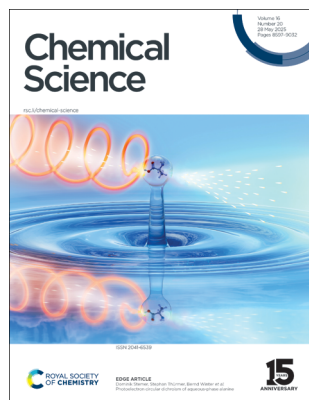


IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 16(20) 8597–9032 (2025)



Cover

See Dominik Stemer, Stephan Thürmer, Bernd Winter *et al.*, pp. 8637–8647. Image reproduced by permission of Dominik Stemer from *Chem. Sci.*, 2025, **16**, 8637. The authors would like to thank Vanessa Shababzadeh for the design and production of the cover illustration.



Inside cover

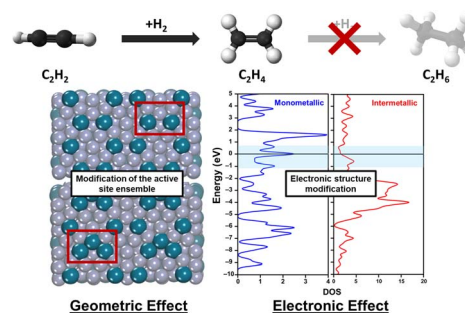
See Haibo Xie *et al.*, pp. 8648–8660. Image reproduced by permission of Haibo Xie from *Chem. Sci.*, 2025, **16**, 8648.

REVIEW

8611

Structural chemistry of intermetallic compounds for active site design in heterogeneous catalysis

Nilanjan Roy, Kathryn MacIntosh, Mustafa Eid, Griffin Canning and Robert M. Rioux*

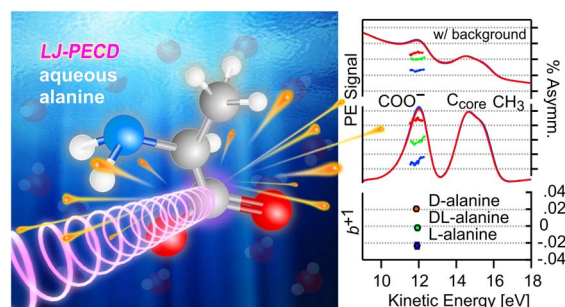


EDGE ARTICLES

8637

Photoelectron circular dichroism of aqueous-phase alanine

Dominik Stemer,* Stephan Thürmer,* Florian Trinter, Uwe Hergenbahn, Michele Pugini, Bruno Credidio, Sebastian Malerz, Iain Wilkinson, Laurent Nahon, Gerard Meijer, Ivan Powis and Bernd Winter*



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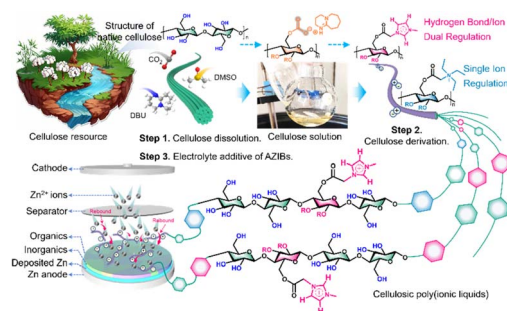
rsc.li/EESCatalysis

**Fundamental questions
Elemental answers**

8648

Design of cellulosic poly(ionic liquid)s with a hydrogen bond/ion dual regulation mechanism for highly reversible Zn anodes

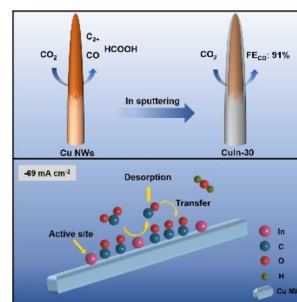
Kui Chen, Yongzhen Xu, Hebang Li, Yue Li, Lihua Zhang, Yuanlong Guo, Qinqin Xu, Yunqi Li and Haibo Xie*



8661

Tuning intermediate binding enables selective electroreduction of carbon dioxide to carbon monoxide on a copper–indium catalyst

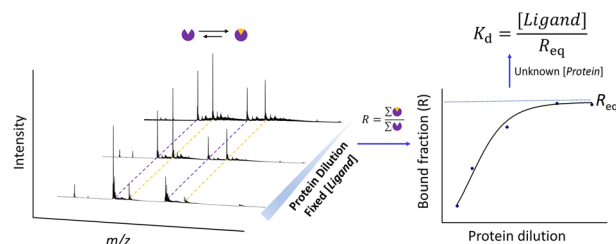
Shengzhou Xu, Chenglong Wang, Chunjing Ran, Hexing Yang, Wangjiang Gao, Bitao Dong,* Yuhang Liu and Dan Ren*



8673

A straightforward method for measuring binding affinities of ligands to proteins of unknown concentration in biological tissues

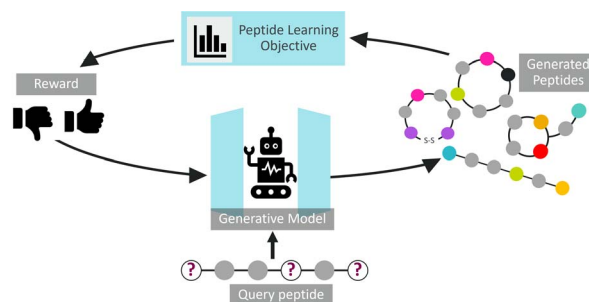
Bin Yan* and Josephine Bunch*



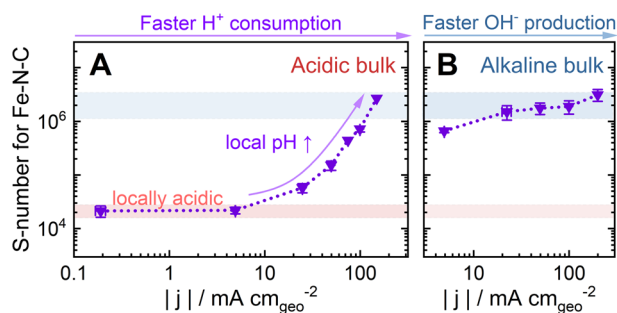
8682

PepINVENT: generative peptide design beyond natural amino acids

Gökçe Geylan,* Jon Paul Janet, Alessandro Tibo, Jiazhen He, Atanas Patronov, Mikhail Kabeshov, Werngard Czechtizky, Florian David, Ola Engkvist and Leonardo De Maria



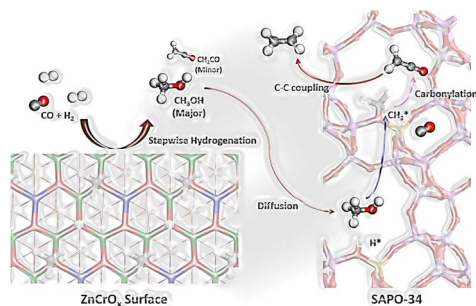
8697



Establishing the stability number descriptor for Fe–N–C fuel cell electrocatalysts

Yu-Ping Ku,^{*} Kavita Kumar, Antoine Bonnefont, Li Jiao, Marco Mazzucato, Christian Durante, Frédéric Jaouen and Serhiy Cherevko^{*}

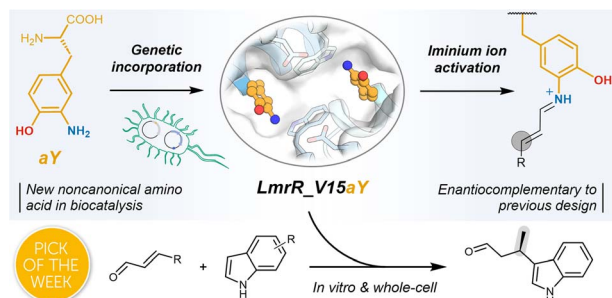
8711



Unraveling the mechanisms of ketene generation and transformation in syngas-to-olefin conversion over ZnCrO_x|SAPO-34 catalysts

Zhuo-Yan Yao, Sicong Ma^{*} and Zhi-Pan Liu^{*}

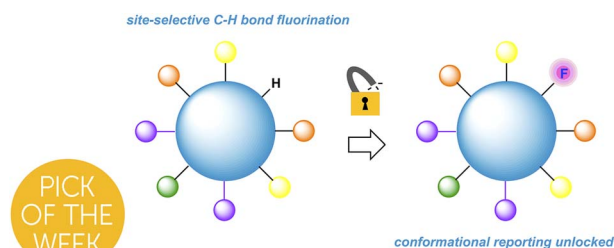
8721



Genetically encoded 3-aminotyrosine as catalytic residue in a designer Friedel–Crafts alkylase

Bart Brouwer, Franco Della-Felice, Andy-Mark W. H. Thunnissen and Gerard Roelfes^{*}

8729



A highly selective C–H bond fluorination unlocks conformational reporting in a complex natural product derivative

Jonah Ruskin, Roxanne Dekeyser, Nathaniel Garrison, Phoebe Williams, Maya Kramer-Johansen, Ananya Majumdar, Travis Dudding,^{*} Adam Huczyński^{*} and Thomas Lectka^{*}

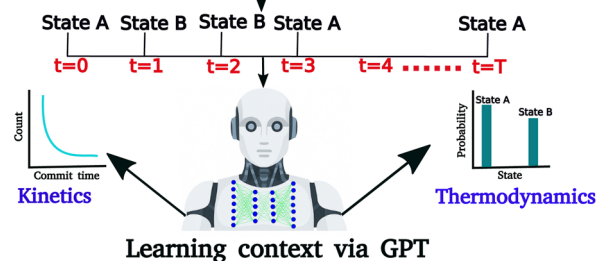


8735

Accurate prediction of the kinetic sequence of physicochemical states using generative artificial intelligence

Palash Bera* and Jagannath Mondal*

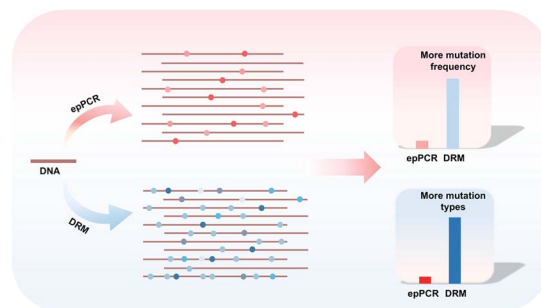
Molecular Dynamics simulation trajectory



8752

Deaminase-driven random mutation enables efficient DNA mutagenesis for protein evolution

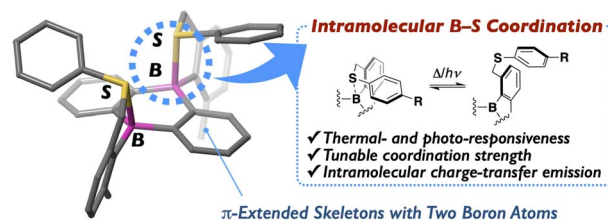
Ying Hao, Tong-Tong Ji, Shu-Yi Gu, Shan Zhang, Yao-Hua Gu, Xia Guo, Li Zeng, Fang-Yin Gang, Jun Xiong, Yu-Qi Feng,* Neng-Bin Xie* and Bi-Feng Yuan*



8764

Intramolecular arylsulfide-coordinated diboraanthracenes: effect of B–S coordination on ground-state and excited-state behavior

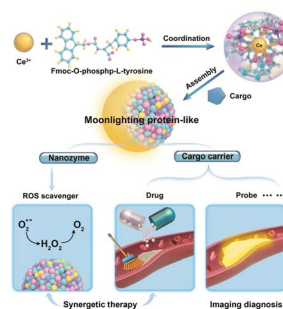
Hiroki Narita, Alexander Virovets, Hans-Wolfram Lerner, Matthias Wagner and Shigehiro Yamaguchi*



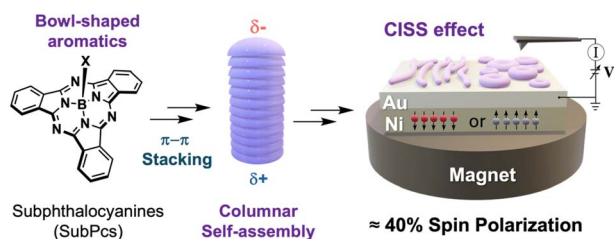
8772

Multifunctional cerium-based nanozymes as moonlighting protein mimics for atherosclerosis diagnosis and therapy

Gui-Mei Han, Jing-Qi Liu, Zhi-Qi Dai, Wei-Liang Jin, Qi-Liang Cai,* De-Ming Kong* and Li-Na Zhu*



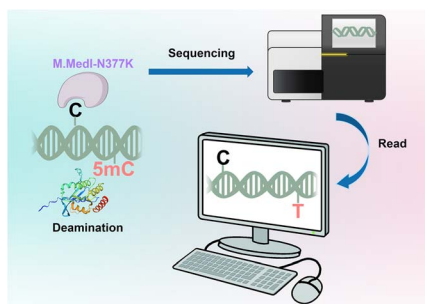
8783



Spin filtering in self-assembled bowl-shaped aromatics

Jorge Labella,* Anu Gupta, Anil Kumar, Elisa López-Serrano, Deb Kumar Bhowmick, Ron Naaman* and Tomás Torres*

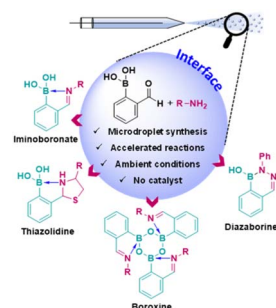
8788



Direct single-nucleotide resolution sequencing of DNA 5-methylcytosine using engineered DNA methyltransferase-mediated CMD-seq

Wei Liu, Zhao-Cheng Ma, Shan Zhang, Fang-Yin Gang, Tong-Tong Ji, Yao-Hua Gu, Neng-Bin Xie, Shu-Yi Gu, Xia Guo, Tian Feng, Yu Liu,* Jun Xiong* and Bi-Feng Yuan*

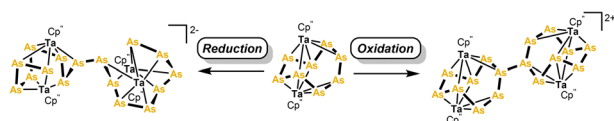
8800



Accelerated click reactions using boronic acids for heterocyclic synthesis in microdroplets

Jyotirmoy Ghosh and R. Graham Cooks*

8807



Redox mediated dimerisation of a cyclo-As₈ complex

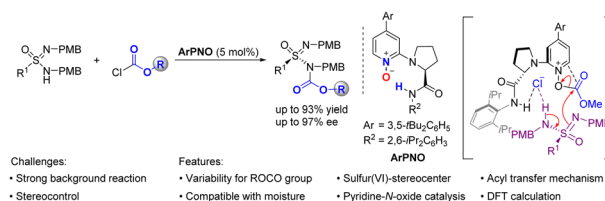
Christoph Riesinger and Manfred Scheer*



8812

Pyridine-*N*-oxide catalyzed asymmetric *N*-acylative desymmetrization of sulfonimidamides

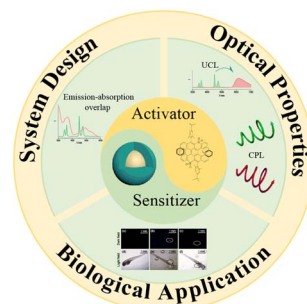
Cui-Mei Guo, Fang-Yuan Zhang, Yin Tian,*
Ming-Sheng Xie* and Hai-Ming Guo*



8820

Boosting near-infrared-triggered photon upconversion in optical nanomaterials via lanthanide-doped nanoparticle sensitization

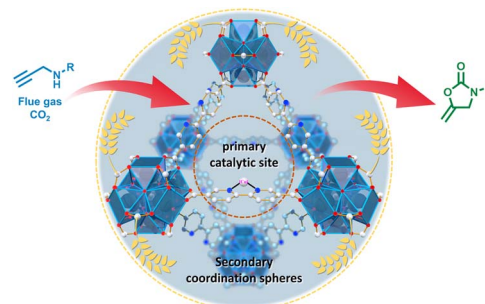
Jiangshan Luo, Junjian Shen, Xingwen Cheng,* Yan Liu,
Xiulian Yin, Tianxi Hu, Guangxin Fan, Jianming Zhang,
Wei Zheng* and Xueyuan Chen*



8827

Tailored engineering of primary catalytic sites and secondary coordination spheres in metalloenzyme-mimetic MOF catalysts for boosting efficient CO₂ conversion

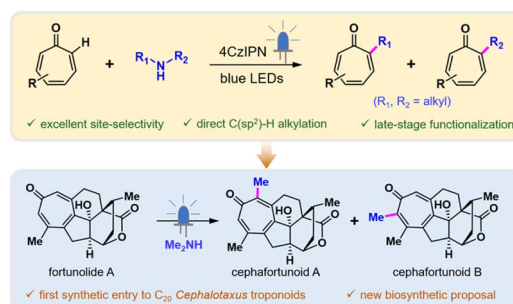
Jiawei Li,* Fan Yang, Benling Yu, Zhongke Dai,
Shiyuan Wei, Ying Wu,* Liuqing He, Fa Zhou,
Jianhan Huang* and You-Nian Liu



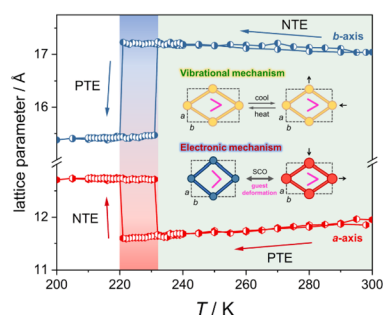
8836

Visible-light-mediated site-selective C(sp²)-H alkylation of tropones facilitates semi-synthesis of cephafortunoids A and B

Qi-Xiang Zeng, Cheng-Yu Zheng, Zhan-Peng Ge,
Jin-Xin Zhao* and Jian-Min Yue*



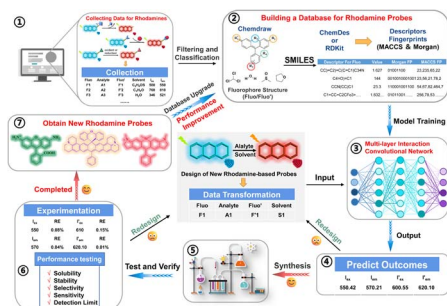
8845



Switchable colossal anisotropic thermal expansion in a spin crossover framework

Si-Guo Wu, Wen Cui, Ze-Yu Ruan, Zhao-Ping Ni* and Ming-Liang Tong*

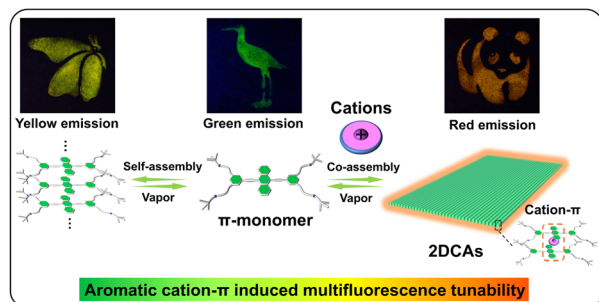
8853



Enhancing fluorescent probe design through multilayer interaction convolutional networks: advancing biosensing and bioimaging precision

Gongcheng Ma, Qihang Ding,* Yuding Zhang, Xiaodong Zeng, Kai Zhu, Hongli Chen, Wenxuan Zhang, Qingzhi Wang, Shuman Huang, Ping Gong,* Zhengwei Xu* and Xuechuan Hong*

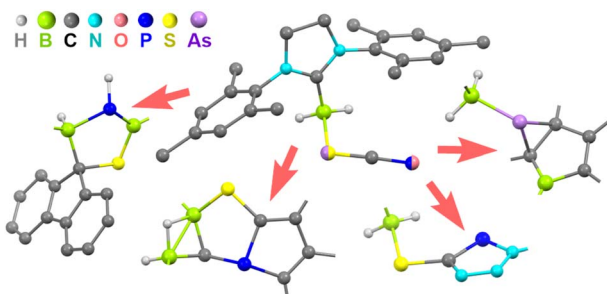
8861



Aromatic cation- π induced multifluorescence tunable two-dimensional co-assemblies for encoded information security

Zhao Gao, Jianxiang Sun, Lulu Shi, Wei Yuan and Wei Tian*

8870



Synthesis and reactivity of a parent phosphathioethynolato-borane and a boraarsaketene

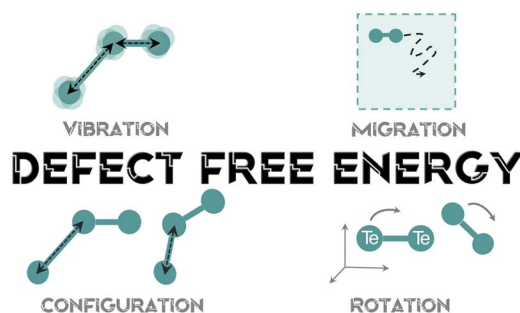
Malte Jürgensen, Tanja Kunz, Merle Arrowsmith, Maximilian Dietz, Stephan Hagspiel and Holger Braunschweig*



8878

Point defect formation at finite temperatures with machine learning force fields

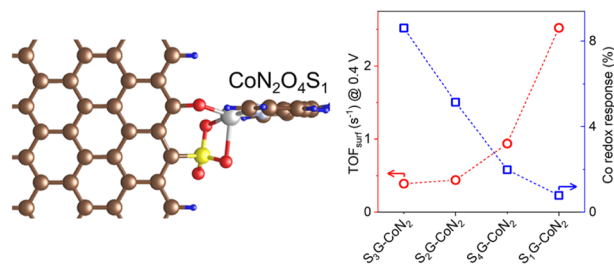
Irea Mosquera-Lois, Johan Klarbring and Aron Walsh*



8889

Tuning the electrochemical redox-mediated mechanism of oxygen evolution on cobalt sites by hydroxide ion coupling

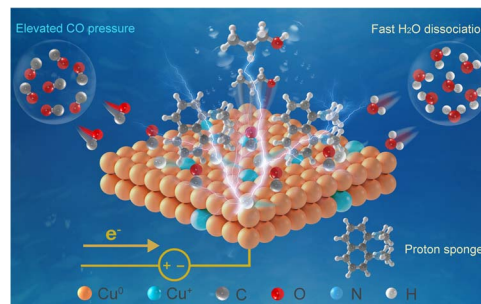
Wenjuan Song, Xiaoyue Duan, Poe Ei Phyu Win, Xiang Huang* and Jiong Wang*



8897

Cooperative promotion of electroreduction of CO to *n*-propanol by *CO enrichment and proton regulation

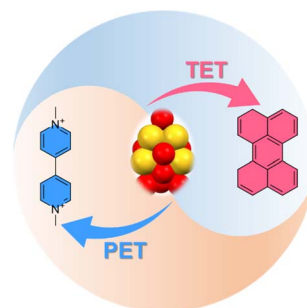
Rongxing Qiu, Linxiao Cui, Li Peng,* Olga A. Syzgantseva, Jiaran Li, Nan Fang, Maria A. Syzgantseva, Yuan Jiang, Jie Zhang, Bingxing Zhang, Lingzhi Ding, Yangyang Dong, Tianwei Xue, Cheng Li, Jin-Chao Dong, Jinyu Ye, Isil Akpinar, Shuliang Yang,* Jun Li,* Jianling Zhang, Jian-Feng Li and Buxing Han*



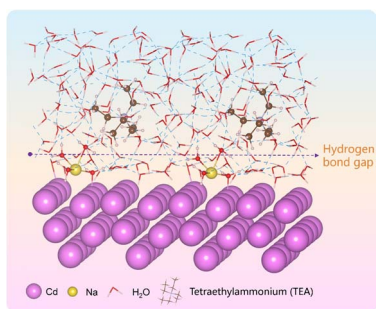
8910

Intensive near-infrared emitting Au₇Cu₁₀ nanoclusters for both energy and electron harvesting

Wei Zhang, Tingting Xu, Jie Kong, Yuanming Li, Xiaoguo Zhou, Jiachen Zhang, Qun Zhang, Yongbo Song,* Yi Luo* and Meng Zhou*



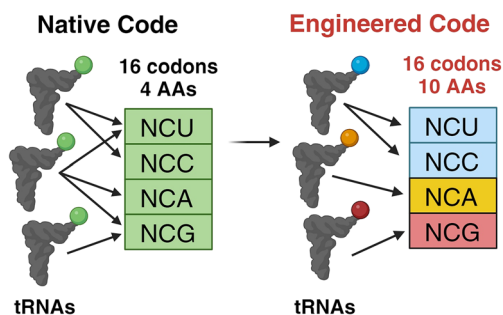
8922



Promotion or suppression of hydrogen evolution activity? The competition between sodium cations and quaternary ammonium ions at the metal/water interface

Shilin Bo, Yang Xiang, Qiong Xiang, Li Li, Xun Huang* and Zidong Wei*

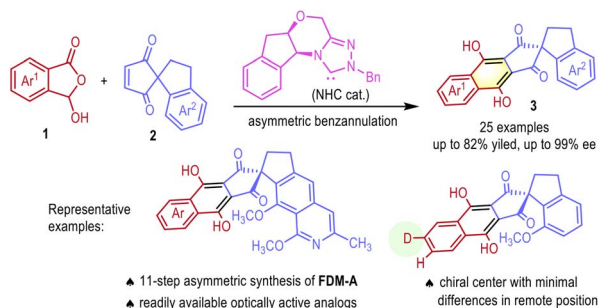
8932



Removing redundancy of the NCN codons *in vitro* for maximal sense codon reassignment

Clark A. Jones, Chelsea A. Makovsky, Aidan K. Haney, Alba C. Dutra, Clinton A. L. McFeely, T. Ashton Cropp and Matthew C. T. Hartman*

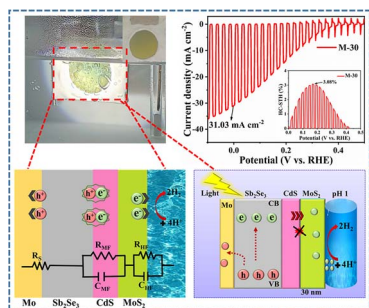
8940



Carbene-catalyzed enantioselective construction of a quasi-symmetrical spirocyclic hydroquinone with a minor chiral distinction

Panlong Ren, Qing Zhao, Yonggui Robin Chi* and Tingshun Zhu*

8946



Pt-free MoS₂ co-catalyst enables record photocurrent density in Sb₂Se₃ photocathodes for highly efficient solar hydrogen production

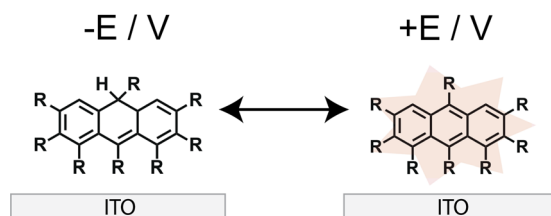
Munir Ahmad, Anadil Gul, Hafiz Sartaj Aziz, Tahir Imran, Muhammad Ishaq, Muhammad Abbas, Zhenghua Su and Shuo Chen*



8959

An investigative study of electrochemical induced fluorescence for fluorophores

Daniel E. Hagness, Ying Yang, Yuanqing Ma, Sumaya Ishtiaq, Sanjun Fan, Richard D. Tilley* and J. Justin Gooding*

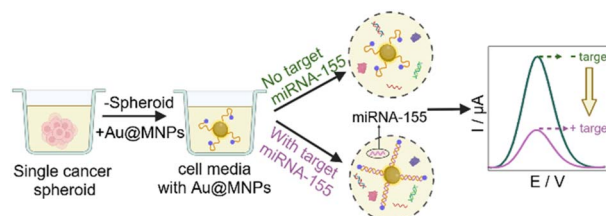


How does fluorophore structure influence the electrochemical modulation of fluorescence?

8970

Direct detection of microRNA in liquid biopsies from single cancer spheroids

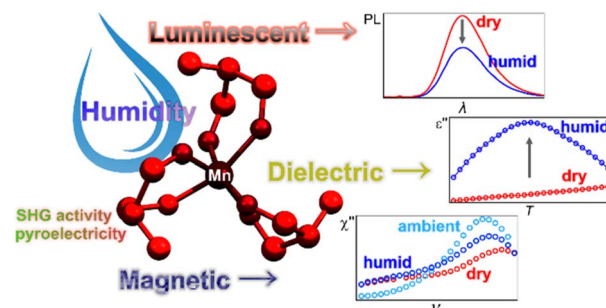
Chen Hu, Essam M. Dief, Bram G. Soliman, Sara Romanazzo, Shilpa Rana, Kristopher A. Kilian, Richard D. Tilley* and J. Justin Gooding*



8979

Photoluminescent, dielectric, and magnetic responsivity to the humidity variation in SHG-active pyroelectric manganese(II)-based molecular material

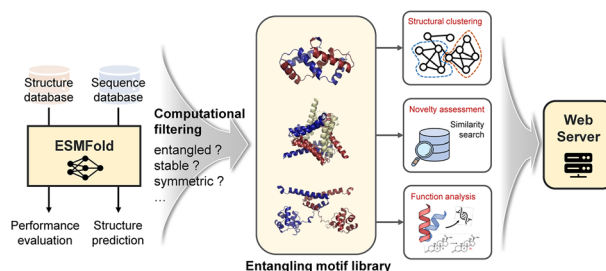
Aleksander Hoffman, Mikolaj Zychowicz, Junhao Wang, Keisuke Matsuura, Fumitaka Kagawa, Jan Rzepiela, Michal Heczko, Sebastian Baś, Hiroko Tokoro, Shin-ichi Ohkoshi and Szymon Chorazy*



8998

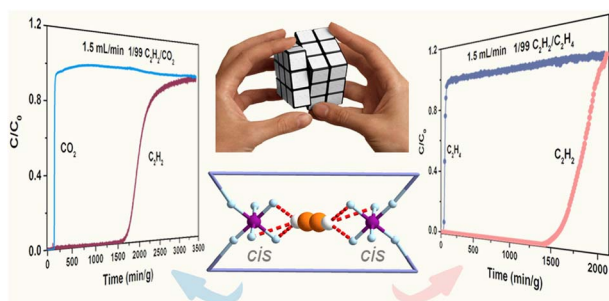
Computational discovery and systematic analysis of protein entangling motifs in nature: from algorithm to database

Puqing Deng, Yuxuan Zhang, Lianjie Xu, Jinyu Lyu, Linyan Li, Fei Sun, Wen-Bin Zhang* and Hanyu Gao*



EDGE ARTICLES

9010



A new type of C₂H₂ binding site in a *cis*-bridging hexafluorosilicate ultramicroporous material that offers trace C₂H₂ capture

Bai-Qiao Song,^{*} Mei-Yan Gao, Lisa Mercene van Wyk, Cheng-Hua Deng, Alan C. Eaby, Shi-Qiang Wang, Shaza Darwish, Dan Li, Shao-Jie Qin, Yun-Lei Peng,^{*} Qing-Yuan Yang, Leonard J. Barbour and Michael J. Zaworotko^{*}

9020



Facile post-synthesis of isomeric covalent organic frameworks *via* precise pore surface engineering

Yuhao Liu,^{*} Yaze Chen, Ke Shi, Haijiao Peng and Chao Lu^{*}

CORRECTION

9029

Correction: A comprehensive approach for elucidating the interplay between 4fⁿ⁺¹ and 4fⁿ5d¹ configurations in Ln²⁺ complexes

Maria J. Beltran-Leiva, William N. G. Moore, Tener F. Jenkins, William J. Evans,^{*} Thomas E. Albrecht^{*} and Cristian Celis-Barros^{*}

